

(FILE 'HOME' ENTERED AT 10:43:51 ON 13 SEP 2006)

FILE 'REGISTRY' ENTERED AT 10:44:01 ON 13 SEP 2006

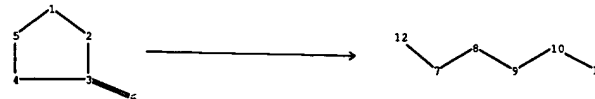
L1	1 S 1,4-BUTANEDIOL/CN
L2	3602 S MALEIC ACID
L3	1 S MALEIC ACID/CN
L4	1 S BUTANEDIOIC ACID/CN
L5	3 S COPPER OXIDE/CN
L6	0 S GAMMA-BUTYROLACTONE/CN
L7	1 S BUTYROLACTONE/CN

FILE 'CAPLUS, CAOLD' ENTERED AT 10:46:40 ON 13 SEP 2006

L8	91 S L1 AND L5
L9	4 S L8 AND L3
L10	45 S L8 AND L7
L11	3 S L10 AND L3
L12	0 S L11 NOT L9
L13	1 S L10 AND L4
L14	1 S L13 NOT L9
L15	27786 S 1,4-BUTANEDIOL OR ?BUTANE-1,4-DIOL
L16	100 S L15 AND L5
L17	0 S L16 AND ?BLACTONE
L18	51 S L16 AND ?LACTONE
L19	28 S L18 AND HYDROGENAT?
L20	19 S L19 AND L7
L21	17 S L20 NOT L9
L22	16 S L21 NOT L14
L23	7 S L22 AND PHASE
L24	9 S L22 NOT L23

FILE 'CASREACT' ENTERED AT 11:21:44 ON 13 SEP 2006

L25	STRUCTURE UPLOADED
L26	STRUCTURE UPLOADED
L27	37 S L25
L28	840 S L25 FUL
L29	6 S L26
L30	132 S L26 FUL
L31	9 S L28 AND L30
L32	0 S L31 AND L5
L33	5 S L27 AND HYDROGENAT?
L34	0 S L33 AND COPPER
L35	803 S L28 NOT L27
L36	112 S L35 AND HYDROGENAT?
L37	7 S L36 AND COPPER
L38	33 S L30 AND HYDROGENAT?
L39	7 S L38 AND COPPER
L40	7208 S 39 NOT L37
L41	7 S L39 NOT L37



chain nodes :

6 7 8 9 10 11 12

ring nodes :

1 2 3 4 5

chain bonds :

3-6 7-8 7-12 8-9 9-10 10-11

ring bonds :

1-2 1-5 2-3 3-4 4-5

exact/norm bonds :

1-2 1-5 2-3 3-4 3-6 4-5

exact bonds :

7-8 7-12 8-9 9-10 10-11

Match level :

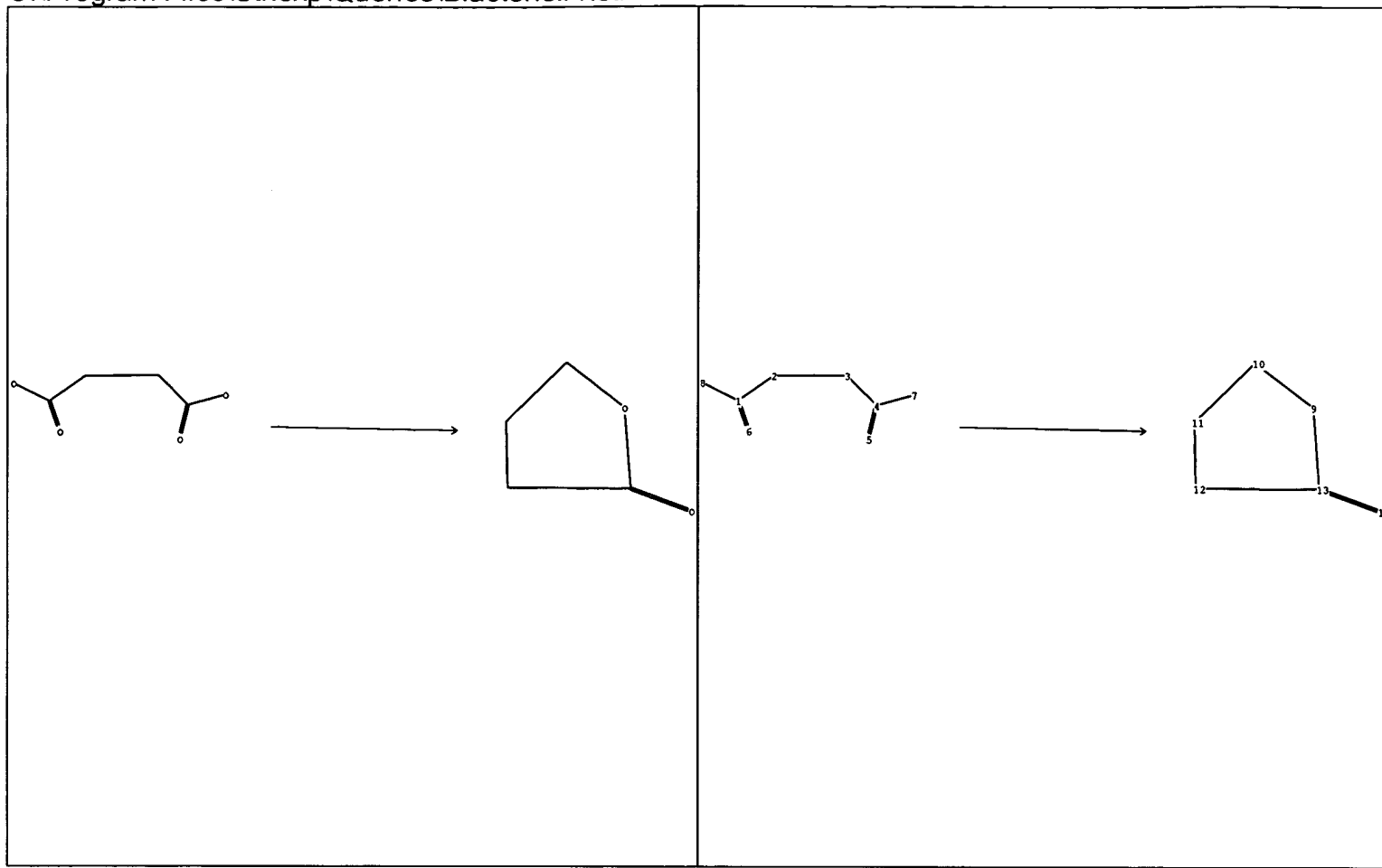
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS7:CLASS8:CLASS9:CLASS10:CLASS11:CLASS  
12:CLASS

fragments assigned product role:

containing 7

fragments assigned reactant/reagent role:

containing 1



chain nodes :

1 2 3 4 5 6 7 8 14

ring nodes :

9 10 11 12 13

chain bonds :

1-2 1-6 1-8 2-3 3-4 4-5 4-7 13-14

ring bonds :

9-10 9-13 10-11 11-12 12-13

exact/norm bonds :

1-6 1-8 4-5 4-7 9-10 9-13 10-11 11-12 12-13 13-14

exact bonds :

1-2 2-3 3-4

Match level :

1:CLASS2:CLASS3:CLASS4:CLASS5:CLASS6:CLASS7:CLASS8:CLASS9:Atom 10:Atom 11:Atom  
12:Atom 13:Atom 14:CLASS

fragments assigned product role:

containing 9

fragments assigned reactant/reagent role:

containing 1